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Optical emissions associated with energetic electrons produced by stepping leaders in cloud-to-ground lightning discharges

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Key Points:
- Optical emissions from energetic electrons produced by lightning leaders
- Predictions on morphological and spectroscopic features of optical emissions
- Using optical emissions to evaluate the electrical properties of lightning leaders

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Abstract Both natural cloud-to-ground and rocket-triggered lightning flashes have been found to be associated with intense and brief bursts of X-ray emissions. Using a full energy Monte Carlo model combined with an optical emission model, we quantify the optical emissions induced by the strong acceleration of thermal runaway electrons in the highly inhomogeneous electric field produced by stepping lightning leaders. The results demonstrate that this acceleration process is accompanied with not only high-energy X-ray emissions but also detectable levels of optical emissions. The fluorescence beam exhibits a conical shape and appears to be larger than the streamer zone associated with the lightning leader. Moreover, we emphasize that the size of the fluorescence beam largely depends on the electrical properties of the associated lightning leader and the intensity ratio between emissions from the second positive band system of N_2 and the first negative band system of N_2^+ reflects the intrinsic difference in the energetics of electrons involved. Therefore, corresponding measurements compared to modeling results can provide useful information for understanding of the stepping mechanism of lightning leaders and associated X-ray production processes.

1. Introduction

Moore et al. [2001] and *Dwyer et al.* [2003] have shown that both natural cloud-to-ground (CG) and rocket-triggered lightning flashes are associated with intense and brief bursts of X-ray emissions. Based on measurements at the International Center for Lightning Research and Testing (ICLRT), it has been further shown that the stepping process in CG lightning leaders is correlated with emission of X-rays [e.g., *Dwyer et al.*, 2005; *Howard et al.*, 2008]. Moreover, measurements by the Thunderstorm Energetic Radiation Array (TERA) and high-speed X-ray camera (XCAM) located at the ICLRT have significantly improved our knowledge about these energetic emissions. *Schaal et al.* [2012] have suggested that TERA measurements can be explained by the propagation of X-rays resulting from bremsstrahlung of energetic electrons with a characteristic energy less than 3 MeV and a production rate on the order of 10^{17} s^{-1}. Additionally, by capturing the spatial structure of X-ray emissions during triggered lightning discharges using XCAM, *Schaal et al.* [2014] have found that the X-ray source region can be compact, with a typical radius between 2 and 3 m, and contains electric charge on the order of 10^{-4} C.

Although extensive ground-based measurements [e.g., *Dwyer et al.*, 2005; *Schaal et al.*, 2012] and modeling studies [e.g., *Dwyer*, 2004; *Moss et al.*, 2006; *Gurevich et al.*, 2007] have been performed, the exact origin of these X-ray emissions is still uncertain. *Dwyer* [2004] has shown that the mechanism of relativistic runaway electron avalanches driven by large-scale thunderstorm electric field is not responsible for this energetic phenomenon, and *Celestin and Pasko* [2011] have proposed that the large fluxes of thermal runaway electrons produced by streamers in stepping lightning leaders in CGs could generate sufficient numbers of X-rays to explain ground-based observations. Further modeling studies reported by *Xu et al.* [2014] have indicated that stepping lightning leaders with electric potentials of 5 MV or 10 MV are able to produce bremsstrahlung photons with energy spectra resembling ground-based measurements. It is also worth mentioning that the energy spectra of gamma rays derived from this mechanism for lightning leaders in intracloud flashes (ICs) are consistent with satellite measurements of Terrestrial Gamma-ray Flashes (TGFs) [e.g., *Xu et al.*, 2012; *Celestin et al.*, 2012].

More recently, high-speed video observations of *Stolzenburg et al.* [2013] have revealed bursts of light during the initial breakdown stage of both CGs and ICs, and the authors suggested that the impulsive breakdown associated with initial leaders causes these light emissions. Spectroscopic analysis of optical emissions is usually used in the studies of Transient Luminous Events (TLEs) to infer the underlying electric field associated with these events [e.g., *Kuo et al.*, 2005; *Liu et al.*, 2006; *Celestin and Pasko*, 2010a]. The purpose of the present work is to quantify theoretically the optical emissions induced by the acceleration process of thermal runaway electrons in the electric field present near the tip region of stepping CG lightning leaders with particular emphasis on the predicted morphological and spectroscopic features.

2. Model Formulation

In this work, we investigate optical emissions originating from the radiative relaxation of excited species of neutral and ionized nitrogen molecules, primarily the second positive band system of N_2 ($C^3\Pi_u \rightarrow B^3\ \Pi_g$) (2P$N_2$) and the first negative band system of N_2^+ ($B^2\Sigma_u^+ \rightarrow X^2\Sigma_g^+$) (1N$N_2^+$). Emissions from these two optical band systems are quantified, from first principles, in the framework of Monte Carlo simulations by modeling dynamically the evolution of excited species. Specifically, similarly to the modeling studies reported by *Xu et al.* [2014], we first use the method of moments [*Balanis*, 1989, p. 670] in order to calculate the electric field produced near the tip region of lightning leaders during the stepping process in CGs. Assuming that seed thermal runaway electrons have been produced by streamer discharges during the negative corona flash stage of a stepping leader [*Celestin and Pasko*, 2011], a Monte Carlo model is then employed to simulate their acceleration in the leader field. Finally, we use an optical emission model accounting for collisional quenching processes and evaluate the resultant optical emissions. In the following, we describe the numerical models used in this study.

Based on detailed simulations of X-ray emissions during the stepping process of lightning leaders, *Xu et al.* [2014] have shown that typical ground-based measurements of X-rays are similar to those produced by lightning leaders with an electric potential of 5 MV. This electric potential drop is therefore chosen in the present study. The electric potential of the lightning leader tip with respect to the ambient potential is approximately $U_l = E_0 l/2$ [*Bazelyan and Raizer*, 2000, p. 54], where E_0 is the ambient large-scale thunderstorm electric field and l is the length of the leader channel. For a potential drop of 5 MV, we assume an ambient electric field produced by the thunderstorm of 0.1 kV/cm [e.g., *Marshall et al.*, 2001]. The length of the lightning leader is considered as 1 km, and the radius of the leader channel is 1 cm [*Rakov and Uman*, 2003, section 4.4.6, p. 134].

The Monte Carlo model used for simulating electrons accelerating in the lightning leader electric field is similar to that described in [*Celestin and Pasko*, 2011], which is three-dimensional (3-D) in the velocity space, 3-D in the configuration space, relativistic, and simulates electrons with energies from sub-eV to GeV. The initial energy of thermal runaway electrons is taken as 65 keV [*Celestin and Pasko*, 2011], and the initial location of these electrons is set to be 15 cm from the leader tip, where the electric field is equal to 27.4 kV/cm. We note that the exact value of the initial energy chosen is not critical as long as the initial electrons are runaway in the leader field. In addition to the high-energy electron simulations, we consistently simulate the production, dynamics, and collisions of low-energy secondary electrons with kinetic energy above 10 eV. We note that the lower limit in energy in our simulations (10 eV) is below the threshold energy for producing N_2 ($C^3\Pi_u$) or N_2^+($B^2\Sigma_u^+$), and thus, the generation of upper excited states responsible for optical emissions from 2PN_2 and 1NN_2^+ is fully modeled.

For the two types of optical emissions considered in the present study, at typical altitudes of CG lightning leaders, the corresponding upper excited states are mostly populated via direct impact excitations by electrons and depopulated via collisional quenching with air molecules. In order to explore the morphological characteristics of the associated fluorescence emissions, the region in the vicinity of the lightning leader tip is discretized using a numerical Cartesian grid of $401 \times 401 \times 401$ grid points, corresponding to a total spatial extent of 8 m in x, y, and z directions. Figure 1a shows an illustration of the simulation domain used for the evaluation of optical emissions. The cube marked in red represents a numerical cell defined in Monte Carlo code for keeping track of the production of excited species (N_2 ($C^3\Pi_u$) or N_2^+ ($B^2\Sigma_u^+$)). One of the advantages that is afforded by the Monte Carlo model is that it is capable of accurately describing and recording the spatial and temporal information on all collisions taking place in the system. Owing to this advantage, the excitation of N_2 ($C^3\Pi_u$) and N_2^+ ($B^2\Sigma_u^+$), especially their production location and time, can be directly derived from

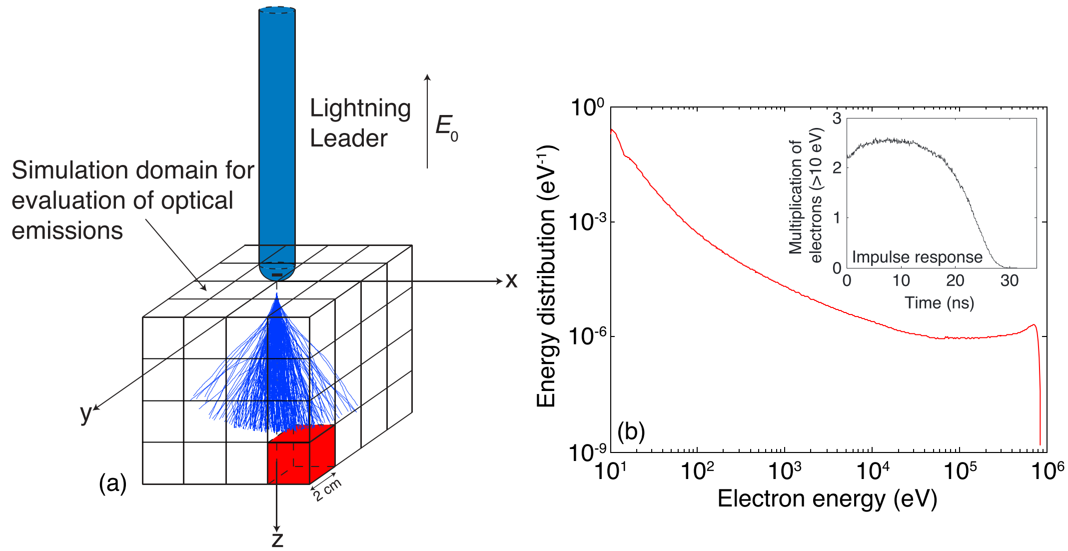

Figure 1. (a) Sketch of the simulation domain used for evaluation of optical emissions. The cube marked in red represents the numerical cell defined for keeping track of the evolution of excited species ($N_2(C^3\Pi_u)$ or $N_2^+(B^2\Sigma_u^+)$); (b) Time-averaged electron energy distribution representing the acceleration process of thermal runaway electrons in the electric field produced during the negative corona flash of a 5 MV lightning leader. The inset shows the multiplication of electrons with energy above 10 eV per electron injected versus time. The results are obtained at ground-level atmospheric density.

Monte Carlo simulations. Concerning the deexcitation of excited species, for each numerical cell defined in the simulation domain (see Figure 1a), we use an optical emission model, similar to that described by *Liu and Pasko* [2004], with an improved set of quenching processes with air molecules (see below) and generation of fluorescence photons via spontaneous emissions. Note that our present calculations do not take into account the effects of radiative transfer between the source of emission and the observer.

For modeling the excitation of N_2 ($C^3\Pi_u$), electron impact excitation cross sections obtained from the BOLSIG+ database [*Hagelaar and Pitchford*, 2005] are used. Moreover, it is considered that N_2 ($C^3\Pi_u$) is deactivated through collisions with N_2 and O_2 molecules with rate coefficients of 10^{-11} cm^3/s [*Kossyi et al.*, 1992] and 3×10^{-10} cm^3/s [*Vallance Jones*, 1974, p. 119], respectively. As for optical emissions from 1NN_2^+, owing to its orbital description of the cross section for ionizing ($2\sigma_u$) electrons from nitrogen molecules, the relativistic binary-encounter-bethe model [*Celestin and Pasko*, 2010b] is used to model the excitation of N_2^+ ($B^2\Sigma_u^+$) [*Van Zyl and Pendleton*, 1995]. The primary quenchers of N_2^+ ($B^2\Sigma_u^+$) are N_2, with a rate coefficient of 4.53×10^{-10} cm^3/s [e.g., *Mitchell*, 1970; *Kuo et al.*, 2005; *Pancheshnyi et al.*, 1998], and O_2, with a rate coefficient of 7.36×10^{-10} cm^3/s [e.g., *Mitchell*, 1970; *Kuo et al.*, 2005; *Pancheshnyi et al.*, 1998]. The optical emission model, along with the set of air fluorescence parameters used in this study, has been validated through comparisons with laboratory experiments [*Xu et al.*, 2015].

3. Results

Figure 1b shows the time-averaged electron energy distribution caused by thermal runaway electrons accelerating in the electric field produced in the tip region of a 5 MV lightning leader. The results are obtained in air at ground-level atmospheric density. The curve is normalized so that the integration over electron energy yields unity, representing the characteristic energy-gaining process undergone by every thermal runaway electron when propagating in the high field region. As shown in this figure, while primary electrons swiftly gain energy in the leader field, secondary electrons with energy greater than 10 eV are also generated along the trajectories, participating to the production of excited species leading to emissions of fluorescence photons. The inset shows the multiplication of electrons with energies above 10 eV per thermal runaway electron injected versus time as an impulse response function of the system. We note that the acceleration process of one thermal runaway electron can lead to a multiplication factor of approximately 2.5 for electrons with energy above 10 eV.

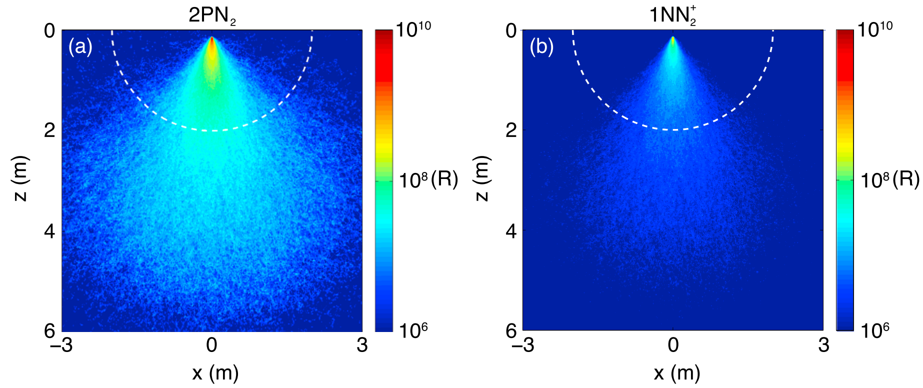

Figure 2. Optical emissions of (a) $2PN_2$ and (b) $1NN_2^+$ resulting from continuous emission of thermal runaway electrons into the 5 MV lightning leader field during the negative corona flash stage, considering an emission rate of 10^{17} s^{-1} [*Schaal et al.*, 2012]. The results are calculated using a convolution technique at ground-level atmospheric density. The dashed lines represent the theoretical size of the associated streamer zone.

Figures 2a and 2b show optical emissions from $2PN_2$ and $1NN_2^+$, respectively, arising from the continuous production of thermal runaway electrons in the electric field of the 5 MV lightning leader by streamer discharges during the negative corona flash stage. Following *Schaal et al.* [2012], we assume that the continuous emission rate of thermal runaway electrons is 10^{17} s^{-1}. The maximum intensities of optical emissions from $2PN_2$ and $1NN_2^+$ are, respectively, 3.2×10^9 R and 4.4×10^8 R. It is important to note that the magnitude of optical emissions depends on the emission rate of thermal runaway electrons. As suggested by *Schaal et al.* [2012], this rate can range from 10^{14} s^{-1} to 10^{17} s^{-1}. Moreover, the emission rate reported by *Schaal et al.* [2012] is not obtained by modeling the dynamics of energetic electrons under the lightning leader field as in the present paper, but using an assumption that the energy distribution of energetic electrons produced by stepped leaders is an exponential function with characteristic energy cutoff. This leads to an uncertainty on the intensities of optical emissions derived in the present work that could be improved by directly comparing our modeling results to observational results. Using Monte Carlo simulations of photon transport to calculate the energy deposition at ground level, we estimate that the relative difference in deposited energy at a radial distance of 50 m obtained between our model (5 MV lightning leader) and an exponential distribution with a characteristic 1 MeV energy cutoff [*Schaal et al.*, 2012] is approximately 24%. This would result in similar differences in the emission rate of energetic electrons and the derived luminosities of optical emissions.

The "irregular" appearance of the emitted light shown in Figure 2 is a numerical feature caused by the limitation in the number of particles modeled in the Monte Carlo simulation and can be improved by increasing the number of particles used at the expense of computation time. We expect that given the true fluxes of thermal runaway electrons, the shape of the fluorescence emissions would be smooth. Moreover, from the linear relationship between the electric potential drop formed in front of lightning leader tips and the radius of associated streamer zone [e.g., *Celestin and Pasko*, 2011], we estimate that the fan-shaped streamer zone present in front of the 5 MV lightning leader would have a radius of 2 m, as marked by dashed lines in Figure 2.

One can estimate that, for a continuous injection of thermal runaway electrons, steady state energy distribution is reached in a few tens of nanoseconds (see inset of Figure 1b). Directly modeling optical emissions associated with the continuous injection of thermal runaway electrons under lightning leader field is computationally expensive because of the large number of numerical cells in energy and configuration space defined in Monte Carlo simulation and the abundant generation of secondary electrons. To overcome this difficulty, we perform a time convolution of the impulse response of the system. Instead of directly modeling the continuous injection, we calculate the temporal evolution of the fluorescence beam corresponding to an ensemble of accelerating thermal runaway electrons in the case that they are all injected simultaneously at $t = 0$ into the lightning leader field (impulse response). Considering that the number of injected thermal runaway electrons is steady and knowing the continuous emission rate, we derive the steady state optical emissions by convolving continuous source with the impulse response over time. We have verified that directly modeling a continuous thermal runaway electron injection leads to results that are consistent with those derived from the convolution technique, but the computation time is significantly prolonged.

The fluorescence beams of $2PN_2$ and $1NN_2^+$, as shown in Figure 2, exhibit a conical shape, similar to laboratory observations of fluorescence from nitrogen at high pressures excited by energetic electrons [*Davidson and O'Neil*, 1964, Figure 1; *Xu et al.*, 2015]. The diameter of this beam is approximately 6 m, as defined by the maximum distance that thermal runaway electrons travel in the leader tip region. In addition, optical emissions of $2PN_2$ are more intense because the frequency of collisional quenching between N_2^+ ($B^2\Sigma_u^+$) and air molecules is much higher at this pressure, even if the excitation rates of N_2 ($C^3\Pi_u$) and N_2^+ ($B^2\Sigma_u^+$) are similar. More importantly, we note that, although optical emissions caused by accelerating thermal runaway electron are much less intense than those from the lightning leader channel, they are spatially separated and spectrally different from those normally produced by lightning leaders [see *Xu et al.*, 2015].

We emphasize that optical emissions induced by thermal runaway electrons largely depend on the electrical properties of the associated lightning leader. For example, in the case of thermal runaway electrons accelerated by the electric field of leaders with an electric potential of 100 MV in intracloud lightning discharges, the corresponding optical emissions have a characteristic radial dimension on the order of a few tens of meters [*Xu et al.*, 2015]. Thermal runaway electrons are capable of gaining more energy from the electric field of lightning leaders with greater electric potentials, corresponding to longer distances propagated and larger fluorescence beams. In addition, the intensity ratio between optical emissions from $2PN_2$ and $1NN_2^+$ is approximately 1.6 [*Xu et al.*, 2015], which is smaller than that of a 5 MV lightning leader as the intensity ratio between $2PN_2$ and $1NN_2^+$ is related to the energetics of electrons involved.

4. Discussion

In this work, using Monte Carlo simulations for electrons with energy above 10 eV, we have studied the dynamics of thermal runaway electrons and their low-energy secondary electrons when propagating in the inhomogeneous electric field produced around the tip region of a 5 MV lightning leader. Using an optical emission model combined with these Monte Carlo simulations, we have predicted theoretically the optical emissions from $2PN_2$ and $1NN_2^+$ associated with the acceleration of runaway electrons.

We have also evaluated the optical emissions associated with thermal runaway electrons by assuming that the large population of high- and low-energy electrons involved in the acceleration process follows a uniform spherical spatial distribution, with a radius of 6 m. The total number of electrons with energy above 10 eV, in the steady state caused by continuous emission of thermal runaway electrons with a rate of 10^{17} s^{-1}, is obtained by convolving the impulse response shown in the inset of Figure 1b. The value is approximately 5.5×10^9. Knowing the energy and number density distributions of electrons, we find that the corresponding intensities of optical emissions from $2PN_2$ and $1NN_2^+$ are, respectively, 5.6×10^{10} R and 7.5×10^9 R. We note that this calculation agrees with modeling results presented in Figure 2 within 1 order of magnitude, and the difference is due to the oversimplification of the electron spatial distribution.

The electric field at the tip of the leader exceeds the electrical breakdown field (~30 kV/cm at ground level), leading to onset of streamer discharges [*Bazelyan and Raizer*, 2000, section 2.4.1, pp. 67–68]. A single streamer first rapidly ionizes air molecules and becomes a space charge wave. In principle, the streamer can then propagate in the form of a narrow filament that can branch into more filaments numerous times. The number of streamers constituting the streamer zone at every moment of time can be estimated using $N_s = Q_s/q_s$, where Q_s is the total electric charge contained in the streamer zone, and q_s is the average charge carried by a streamer, typically on the order of 1 nC [*Bazelyan and Raizer*, 2000, pp. 69–71]. As pointed out by *Celestin and Pasko* [2011], Q_s is quadratically dependent on the electric potential difference formed by lightning leaders with respect to ambient potential (U_l) and can be calculated using $Q_s = \frac{\pi\epsilon_0 U_l{}^2}{2E_s^-}$, where E_s^- is the electric field in the steamer zone of negative leaders and its value is taken as 12.5 kV/cm [*Babaeva and Naidis*, 1997, Figure 7]. From these relations, we estimate that, for the streamer zone associated with a 5 MV lightning leader, the total number of streamers is approximately 3×10^5.

In order to estimate optical emissions radiated from the streamer zone of a 5 MV lightning leader, modeling results of a well-developed negative streamer propagating in a homogeneous field of 20 kV/cm at 14.5 ns after its ignition are used. These results had been obtained in a parametric study performed in preparation of the work reported by *Celestin and Pasko* [2010a] (see this work for further information on the model and the exact simulation configuration and parameters). Note that, at this stage, the radius of the streamer head is approximately 0.13 cm and excited species are mainly concentrated in the head. Knowing the number of streamers, we first calculate the total amount of excited species in the streamer zone. The number density of excited species in the streamer zone is further derived by assuming that they follow a uniform spherically symmetric spatial distribution with a characteristic radius representing the dimension of the streamer zone. Finally, we calculate the corresponding optical emissions and found that the intensities are 4.8×10^{11} R and 7.6×10^{8} R for $2PN_2$ and $1NN_2^+$, respectively. The results show that optical emissions from the streamer zone are 1 order of magnitude more intense than those associated with accelerating thermal runaway electrons. We note that varying the ambient electric field in streamer simulation from 20 kV/cm to 10 kV/cm can lead to a reduction of the intensity by a factor of approximately 7.7.

There are notable differences between optical emissions associated with thermal runaway electrons and those from the streamer zone. First, fluorescence light stemming from thermal runaway electrons accelerating in lightning leader field is estimated to take place over a larger region than that occupied by the streamer zone (see Figure 2), although the luminosity is weaker. Furthermore, considering that the capability of electrons in generating fluorescence photons from $2PN_2$ and $1NN_2^+$ is highly energy dependent [*Xu et al.*, 2015], the intensity ratio between $2PN_2$ and $1NN_2^+$ is related to the energetics of electrons involved. Since electrons in streamer discharges and those produced by thermal runaway electrons follow different energy distributions, this ratio would be inherently different between these two processes. For instance, using the results obtained with a uniform distribution of the excited species (see above), we find that the ratio of the intensity of $2PN_2$ to that of $1NN_2^+$ corresponding to the acceleration process of thermal runaway electrons is approximately 7.5, whereas this quantity is approximately 633 for the associated streamer zone. We note that the quenching scheme considered in the present study is different from that used in the streamer simulation of *Celestin and Pasko* [2010a]. Collisional quenching interactions of N_2 ($C^3\Pi_u$) by N_2 molecules and $N_2^+(B^2\Sigma_u^+)$ by O_2 molecules are not included in these streamer simulations and we have verified that these processes can increase the intensity ratio associated with the streamer zone by approximately 40%. Spatially resolved measurements of the ratio between the intensities of $2PN_2$ and $1NN_2^+$ should therefore provide insightful information for understanding of the associated X-ray production.

Besides the above mentioned differences, one can expect that optical emissions resulting from accelerating thermal runaway electrons are temporally separated from those of the streamer zone. Thermal runaway electrons should be mostly produced during the early establishment of the streamer zone, namely, the negative corona flashes. At this stage, thermal runaway electrons promptly propagate in the high field region and the associated fluorescence beam rapidly expands on a timescale of ∼30 ns. However, the streamer zone is not formed until the space charge field produced by propagating streamers lowers the electric field in the streamer zone down to the stability field of negative streamer propagation (∼12.5 kV/cm) [e.g., *Bazelyan and Raizer*, 2000; *Celestin and Pasko*, 2011]. The typical duration of this process is on the order of ∼1 μs [e.g., *Moss et al.*, 2006]. Indeed, a streamer with a velocity of 10^6 m/s propagates over 2 m (see Figure 2) in 2 μs. It is thus conceivable that measurements would capture the expanding fluorescence beam produced by accelerating thermal runaway electrons followed by more intense optical emissions from the developing streamer zone.

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